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Assisting users on model selection in small angle neutron scattering experiments

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Nowadays software for Small Angle Scattering (SAS) data fitting have a large selection of analytical and numerical models to describe the form factor of the scattering objects. It may become overwhelming to choose an adequate model for the data, especially for new users of SNS instruments. In this work, we train a convolutional neural network (CNN) to predict the form factor model on a dataset comprising of 300.000 SANS 2D images obtained by means of virtual experiments. The CNN hast a 94% of accuracy in the classification task, and a 99.9% top 3 accuracy, i.e. that the probability of the model not being amongst the 3 recommended models (out of the 47 in the database) is 0.1%. We explain the dataset creation, and the training procedure. Once trained, these algorithms can run on the fly, while performing measurements on an instrument. We also show the use of explainable machine learning algorithms, in particular SHAP and Grad-CAM, to interpret how the CNN is making decisions.

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